Topological structure effect on far-infrared spectra in a GaAs/InAs nanoring*

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On the basis of the growth mechanism of a GaAs/InAs nanoring, we propose a fine model which reflects the confinement details of real nanoring. Through calculations of the two-electron energy and far-infrared (FIR) spectra, we find that the ring topological structure and electron-electron interaction have great influence on the FIR spectra. The two unknown transition peaks in the experiment are determined theoretically. The theoretical results are in good agreement with the experiments.

Keywords: nanoring, topological structure, far-infrared spectrum, confinement potential

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1. Introduction

Since a GaAs/InAs nanoring (NR) was prepared successfully and its energy level structure and optical properties were measured by Lorke *et al.*,[1−4] the study of NRs has attracted much attention. The NR, which is different from the mesoscopic ring, is grown by the self-assembly method, and its thickness is only about 2 nm, with an inner radius of 10 nm, and an outer radius of 30–70 nm. In such a small ring structure, carriers behave as completely quantized particles owing to the strong confinement. From the NR experimental results of the capacitance spectra, the two-electron far-infrared (FIR) spectra, and the photoluminescence (PL) spectra of excitons and charged excitons, it can be seen that the energy level structures and optical transitions show the characteristics of ring structures. Compared with quantum dots, NRs have more kinds of optical spectrum structures and richer physics, for example, the Aharonov–Bohm (AB) oscillations[5] with the external magnetic field. Therefore, investigation of NRs has important value not only for basic physics but also for applications of nanodevices.[6]

In order to explain and investigate the electrical and optical characteristics of NRs, researchers have produced many works,[7−11] which involve the electronic structures, optical properties, and transport properties. A profound understanding of the quantum characteristics of NRs from different angles has been given. However, so far, the theories cannot give comprehensively explanations about the experimental results. For example, the origin of some FIR peaks still has not been determined, and PL spectra of excitons and charged excitons still lack rational theoretical analysis. The origin of problems is associated with the inaccuracy of potential models used in theoretical calculations. Compared with the quantum wells and dots, the NR has a more complex topological structure, in which the carriers are not only confined strongly in the width direction but also confined by the inner and outer interfaces in the plane of the ring. In the ring structure, the roughness of the confinement potential in the material interface may have an important effect on the movement of carriers. Therefore, the theoretical model of the potential is required to appropriately describe the ring feature of the confinement potential as well as to reflect the details of component changing in the material interface. The potential models used in some previous NR theoretical calculations, for example, one/two-dimensional and parabolic ring models, are too simple to quantitatively study the quantum characteristics of NRs. Three-dimensional potential models[9,12] were used in some theoretical calculations, but the results of the calculations are not in good agreement with the experimental results due to the failure to describe the details of the NR structure. In this paper, we propose a fine ring po-

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tential (FRP) model which can better meet the true situations. In this model, through calculating the two-electron energy and FIR spectra, we reveal the effects of the topological structure of the NR and electron–electron interaction on the FIR spectrum, and confirm the origin of two unknown transition peaks in the FIR spectrum. On the calculation method side, we use the partitioning series expansion method to exactly solve the intrinsic equation of a single particle for different confinement potentials. Then we employ the accurate diagonalization method to treat the electron–electron interaction, and obtain the eigenvalues and eigenstates of the system.

2. Fine model of an InGaAs nanoring

In previous theoretical studies on NRa, one usually employed the ring-shape potential models based on a two-dimensional square-well and an eccentric parabolic-well. Unfortunately, the square-well potential model is only a qualitative model, and the eccentric parabolic potential (EPP) model faces some difficulties when it is employed to describe the ring-shape confinement. The EPP model cannot give an appropriate height of the central barrier, effective radius, and width at the same time. When the radius of the NR is not very large, the EPP model gives an underestimated central barrier, in which carriers can tunnel the central barrier with a large probability, so the model loses the characteristics of the ring structure. Since the central barrier plays an important role in the ring structure, the ring model should give a correct central barrier height.

In Fig. 1, we display the two-electron FIR absorption spectra of the two kinds of ring-shape potential models in magnetic field. One is the EPP $U(r) = mw^2(r - R_0)^2/2$ (where m is the electron effective mass, and R_0 is the radius of the model potential), and the other is the potential with an additional central barrier. The insets in Fig. 1 give the patterns of the potentials and the radial wave functions of the ground states. It is obvious that the distribution of the wave function in the potential with an additional central barrier has the complete feature of ring-shape confinement, but that in the pure EPP has mainly the feature of dot confinement. Comparing

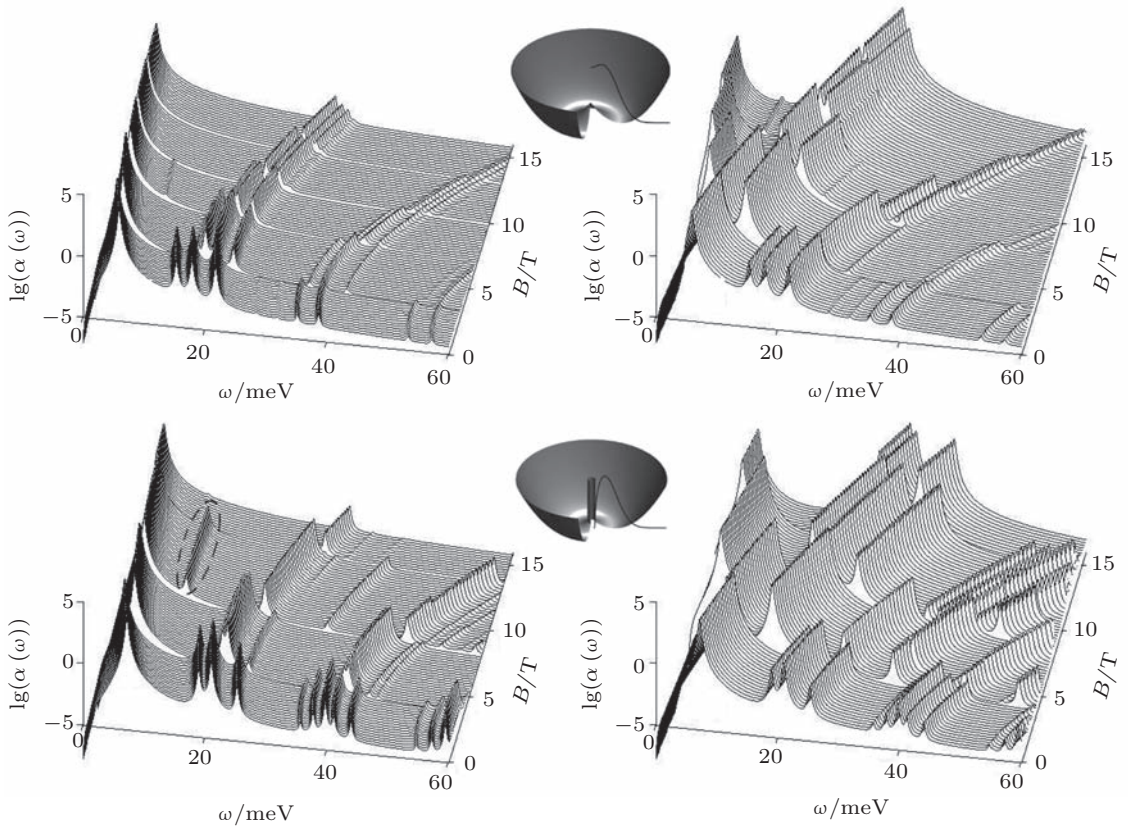


Fig. 1. The two-electron FIR absorption spectra as functions of confining strength ω of model potential and magnetic field B. (a) EPP, and (b) EPP with an additional central barrier. The left and right panels correspond to the left rotating and right rotating light transitions, respectively. Insets are the patterns of the two kinds of potentials and the wave functions of the ground states.

Fig. 1(a) with 1(b), one can see that the complete ring confined potential gives more abundant FIR spectra. Especially, the position of the transition peaks labeled with the dashed line agrees approximately with the unknown experimental peaks.[3] Therefore, the diversity of confinement potential structure strongly influences the calculation results of NR. A perfect ring potential model should have appropriate barrier heights on the inner interface and outer interface to distinguish the ring features from the dot features.

Observing the InGaAs semiconductor NR preparation process,[12] we find that InGaAs NRs come from the shape transformation of InAs/GaAs quantum dot. It is seen from the formation process and structure characteristics that InGaAs NR is a very flat quasi two-dimensional structure. Since the thickness of the ring is very small, carriers move mainly in a local ring plane, and the barrier jump at the interface may affect the carrier movement. Therefore, in the frame of the effective mass, the potential model should have the feature of step structures in order to reflect the interface details. Planelles *et al.*[9] and Voskoboynikov *et al.*[10] also mentioned a similar view. In order to reflect the fine structure of InGaAs NRs, our FRP model is a piecewise continuous function to construct a confined potential with many parameters, and the expression is as follows:

$$U(r) = A_i(r - R_i)^{N_i} + B_i, \tag{1}$$

where A_i, R_i, N_i and B_i are the modulation parameters of every piecewise potential function. The potential step structure can be realized through modulating the value and sign of the potential function power N_i and N_{i+1} of adjacent segments. In our calculations, we take $N_i = 4$ and $N_{i+1} = -4$. The central barrier height and location of each step of FRP can be controlled by the parameters of the piecewise continuous potential function. We draw the pattern of this potential model and the change curve with ring radius, as shown in Fig. 2, in which the EPP is also drawn for convenience of comparison. Compared with the whole of FRP, the change caused by the steps is tiny, which is consistent with the composition gradation of InGaAs NR. However, this tiny change of confined potential has a significant impact on the electronic structure of the NR, which is clearly shown by the complex energy level distribution in the inset of Fig. 2(b). This non-uniform level distribution reflected on FIR transitions results in an abundance of FIR spectra. One can finely adjust the inner radius, outer radius, height, and location of the step potential to make the theoretical calculation comprehensively meet the experimental measurement of the energy spectra and FIR spectra, as well as to obtain the optimal FRP. In addition, the inside and outside effective radiuses of the FRP used in our calculation are consistent with the real InGaAs NR size. Therefore, the FRP model described by Eq. (1) is rational, which can be used in the quantitative calculation of InGaAs NR.

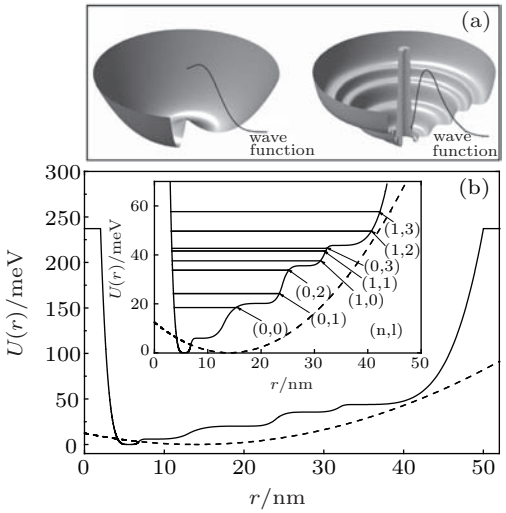


Fig. 2. The patterns of EPP and FRP, and the radial wave function of the ground state. (b) The FRP (solid line) in comparison with EPP (dashed line). The inset in (b) is the zooms of the bottoms of two potentials and the distribution of single electron energy levels of the FRP (horizontal line), where the numbers in the brackets are the quantum numbers of the energy levels.

In Lorke's experiment, there were a lot of rings in his measured samples. However, the inter-ring distance is larger than the electron distribution within the single ring, so the inter-ring coupling can be ignored. See the analysis of Lorke for detail.[12]

3. Energy and FIR spectra in a ring with features of the real structure

With the FRP model, we are able to explore the real structural features of the electronic structure and FIR transitions. In order to solve the intrinsic equation of a single particle in the more complex confined potential, we further improved the partitioning series expansion method, and enabled it to solve

the single-particle intrinsic problems for general segment of power series potential. Combining the diagonalization method,[13] one can accurately obtain the two-electron bound states in the FRP.[14] Since the density of electron is small, the calculation without self-consistency can give an accurate result for a few-electron ring. The bound state of two electrons can be written as follows:

$$\Phi(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2) = \sum_{n_1 l_1, n_2 l_2} A_{n_1 l_1, n_2 l_2} \psi_{n_1 l_1, n_2 l_2}(\boldsymbol{r}_1, \boldsymbol{r}_2)\chi_{\rm s}(\sigma_1, \sigma_2), \quad (2)$$

where $\psi_{n_1 l_1, n_2 l_2}$ is symmetric or anti-symmetric wave function in two-electron space, $\chi_{\rm s}(\sigma_1, \sigma_2)$ is the spin wave function, and n_1, l_1, n_2, l_2 are radial and angular quantum numbers of a single particle. Figure 3 shows that the single-electron and two-electron energy levels change with magnetic field in the FRP model, in which the experimental measurement of single-electron and two-electron ground state energy under the magnetic field is also drawn.

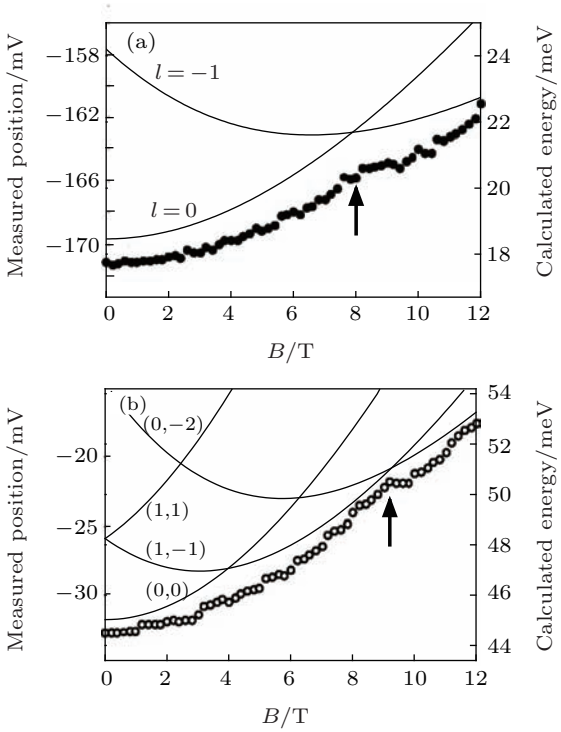


Fig. 3. Variations of single- (a) and two-electron (b) energy levels with magnetic field. Black and white circles are measurement data of single electron and two-electron ground state energy extracted from Lorke *et al.*,[12] respectively. The arrows indicate the oscillating points in magnetic field.

It is obvious that the curve of our theoretical calculation is very consistent with the experimentally measured result. In the single-electron case, theoretical calculations show that the ground state transforms from the state with zero angular momentum ($l = 0$) to the state with the angular momentum ($l = -1$) in $B = 8$ T, and the experimentally measured curve also has a distinct mutation in the slope of the magnetic field. The two-electron ground state under the magnetic field has a clear oscillation phenomena between the singlet state and the triplet state, whose exchange points are at $B = 4$ and 9 T. It can be seen from the experimental measurement that there is a clear turning point for the curve of two-electron ground state at about 9 T. It is worth mentioning that one can approximately obtain the above result by using the EPP model,[7] but must take respectively the different parabolic potential parameters for single-electron and two-electron calculations. However, in experiments the single- and two-electron capacitance spectra are measured in the same sample. Thus, the single-electron and two-electron calculations should be completed in the same confined parameters. By contrast, this FRP model is more realistic.

In order to analyse the FIR transition characteristics of NRs, we give single- and two-electron light transitions under a magnetic field in Fig. 4, in which ω_- and ω_+ represent the left- and right-handed rotation polarized light respectively. The single-electron transition satisfies the selection rules $\Delta l = \pm 1$, corresponding to $\Delta n = 0$ and 1, so there are four possible transitions in the low energy region. With the change of the magnetic field, the exchange of single-electron ground state occurs, and the transition state also changes accordingly. Since the relative and centre of mass motion of the two electrons in NR are inseparable, the FIR transitions do not satisfy Kohn theorem,[15] which is different from the case of the parabolic quantum dots. The ring confinement combines with the correlation of electrons to make the transition probability between two-electron states greatly increase. In Table 1, we list spins, total orbital angular momentums, and the main components of the two-electron states participated in the transitions. Combining Fig. 4(b) and Table 1, one can easily find that the two-electron transitions occur between the same spin states, and when the spin of ground-state oscillates with the magnetic field, the two-electron FIR transition periodically varies accordingly. The ring topological structure and electron–electron interaction make two-electron states contain more single-electron occupied orbits, so the two-electron states in NR have more FIR transition selections.

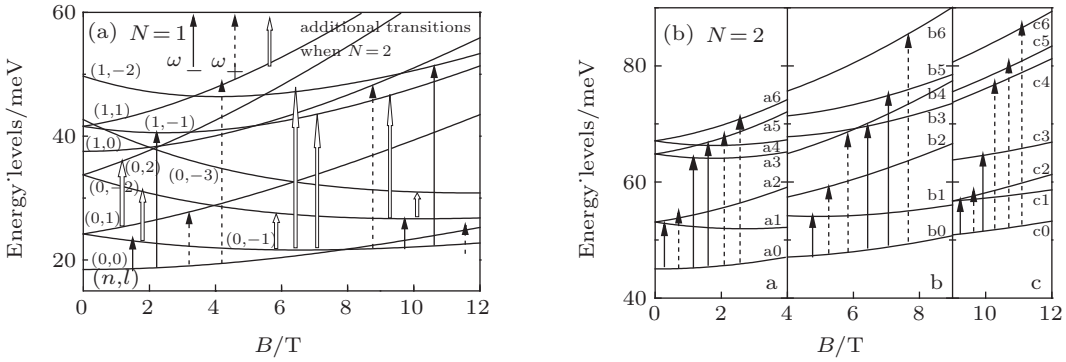


Fig. 4. (a) Single-electron and (b) two-electron absorption transitions changing with the external magnetic field, where ω_- (solid-line arrow) and ω_+ (dotted-line arrow) respectively indicate right- and left-handed rotation light transitions. The hollow arrow indicates the additional transition in two-electron model. The quantum number (n, l) labels the single-electron quantum state, and a_i b_i and c_i label the two-electron quantum states.

Table 1. The spin (S), total orbital angular momentum ($L = l_1 + l_2$), and the main components of the two-electron state (Φ) in the NR.

$\Phi(S,L)$	$(n_1,l_1,n_2,l_2)\lvert A\rvert^2$	$\Phi(S,L)$	$(n_1,l_1,n_2,l_2)\lvert A\rvert^2$	$\Phi(S,L)$	$(n_1,l_1,n_2,\ l_2)\lvert A\rvert^2$
$\mathrm{a}_0(0,0)$	$(0,0,0,0)0.88$, $(0,\text{-}1,0,1)0.10$	$\mathrm{b}_0(1,-1)$	$(0,0,0,-1)0.99$	$\mathrm{c}_0(0,-2)$	$(0,0,0,-2)0.78$, $(0,-1,0,-1)0.21$
$\mathrm{a}_1(0,-1)$	$(0,0,0,-1)0.86$	$\mathrm{b}_1(1,-2)$	$(0,0,0,-2)0.98$	$\mathrm{c}_1(0,-3)$	$(0,-1,0,-2)0.62$, $(0,0,0,-3)0.37$
$\mathrm{a}_2(0,1)$	$(0,0,0,1)0.86$	$\mathrm{b}_2(1,0)$	$(0,-1,0,1)0.99$	$\mathrm{c}_2(0,-1)$	$(0,0,0,-1)0.89$
$\mathrm{a}_3(0,-1)$	$(0,0,1,-1)0.49$, $(0,-1,1,0)0.33$	$\mathrm{b}_3(1,-2)$	$(0,-1,1,-1)0.87$	$\mathrm{c}_3(0,-3)$	$(0,0,0,-3)0.59$, $(0,-1,0,-2)0.32$
$\mathrm{a}_4(0,-1)$	$(0,1,0,-2)0.65$	$\mathrm{b}_4(1,0)$	$(0,0,1,0)0.97$	$\mathrm{c}_4(0,-1)$	$(0,1,0,-2)0.50$, $(0,0,1,-1)0.28$
$\mathrm{a}_5(0,1)$	$(0,0,1,1)0.49$	$\mathrm{b}_5(1,-2)$	$(0,0,1,-2)0.92$	$\mathrm{c}_5(0,-1)$	$(0,0,1,-1)0.31$, $(0,-1,0,-2)0.35$
$\mathrm{a}_6(0,1)$	$(0,-1,0,2)0.65$	$\mathrm{b}_6(1,0)$	$(0,-1,1,1)0.98$	$\mathrm{c}_6(0,-1)$	$(0,-1,1,0)0.54$, $(0,0,1,-1)0.34$

Notes: $S = 0$ and 1 correspond to the spin singlet-state and triplet-state respectively. $|A|^2$ is the expansion coefficient norm of the quantum state, and (n_1, l_1, n_2, l_2) is a combination of one-electron quantum numbers in the Hilbert bases. The labels of the states are the same as those in Fig. 4(b).

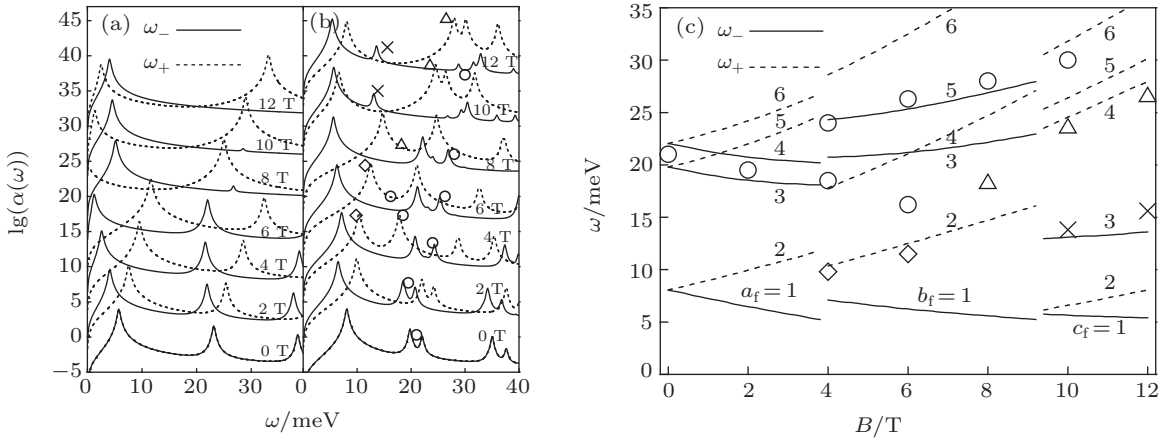


Fig. 5. The two-electron FIR absorption spectra calculated by using EPP model (a) and FRP model (b) in different magnetic fields, and the peak heights of two-electron spectra versus magnetic field (c). Symbols with different shapes represent the experimental data points.[3] The numbers of a_f, b_f, and c_f label three groups of the excited states.

In Fig. 5, we plot the single- and two-electron FIR absorption spectra in some magnetic fields, and the peaks of two-electron spectra change with the magnetic field. Figures 5(a) and 5(b) show that there is a large difference between the single- and two-electron FIR spectra. Therefore, in experiment the two kinds of FIR spectra of NRs should be clearly distinguishable. Compared with the single-electron case, the two-electron FIR spectra of NRs clearly show the periodic oscillations of spin singlet- and triplet-state, and richer spectral structures. It can be seen from Figs. 5(b) and 5(c) that the theoretical calculation concides quantitatively with the experiment, and the peak (x) has a clear attribution, which has not been confirmed by

theoretical calculations. Therefore, the structural details of ring confined potential have a significant impact on FIR optical properties of NRs.

4. Conclusion

In summary, we have proposed a realistic FRP model of NRs through careful analysis of InGaAs NR preparation in experiment. This model has an appropriate height of central barrier, as well as the full ring structural potential, in which the step potential better reflects the structural details of InGaAs NR. Under the same parameters of the FRP model, we have calculated energy spectra, and FIR spectra for the single-electron and two-electron system, which are in quantitative agreement with the experiment. In addition, we have confirmed the origin of two unknown FIR peaks. We find that the InGaAs NR topological structure has an important effect on the quantum properties. For example, the topological structure may sensitively affect the electronic level structure of NR and the AB oscillations of its ground state with the magnetic field. In addition, the topological structure effect combines the electron–electron Coulomb interaction and the magnetic Zeeman effects to make the two-electron FIR transition probability increase greatly, as well as enriching the NR FIR spectra.

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